

Electronic Supplementary Information (ESI) for

First- and second-sphere contributions to Fe(II) site activation by cosubstrate binding in nonheme Fe enzymes

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Computational Details

All calculations were performed using the Gaussian09 computational package.¹ The active sites of α KG-bound FIH in the presence and absence of substrate were modeled using crystal structures of the appropriate forms (PDB ID's 1H2L and 1H2N, respectively) as starting points.² The FIH active site and CAD substrate were truncated as shown in Figure S1A. Carbon atoms shown as spheres were converted to methyl groups and frozen during geometry optimizations. The carbons are as follows: The δ C for α KG, the β C's of His199 and His279, the δ and guanidinium C's of Arg238, the carbonyl C of Asp201, and the α C of Tyr200 for FIH, and the α C's of Val802 and Ala804 for CAD. In model N803G the side chain of CAD Asn803 is replaced with an H atom, in N803A with a methyl group, and in N803A* with a methyl group which is frozen during geometry optimizations. For structures where the full CAD Asn803 was used the model included Gln239 up to the β C, and the backbone amide unit of Pro197, with all terminal C's frozen as shown in Figure S1B. (The Pro197 fragment is used to help keep His199 properly positioned) For the structure with Asn205 and Asn294, the amide groups of these residues were included up to the β C, which was frozen. Geometry optimizations, frequency calculations and single point calculations were conducted using the spin-unrestricted BP86 functional^{3, 4} with 10% Hartree-Fock mixing using the keyword IOP(3/76=0900001000). All calculations were performed under tight convergence criteria. Optimized water-coordinated 6C structures were used as starting points for the 5C structures with the water ligand removed. The triple- ξ basis set 6-311G*⁵⁻⁸ was used to describe the Fe atom, the N and O atoms of the facial triad directly coordinated to Fe, the O atom of both coordinated and dissociated water, and the OC-CO₂ moiety of coordinated α KG, while all other atoms were modeled using the double- ξ basis set 6-31G*.⁹⁻¹³ Solvation effects were included in all calculations through the use of the polarized continuum model (PCM)¹⁴ with a dielectric constant $\epsilon = 4.0$.

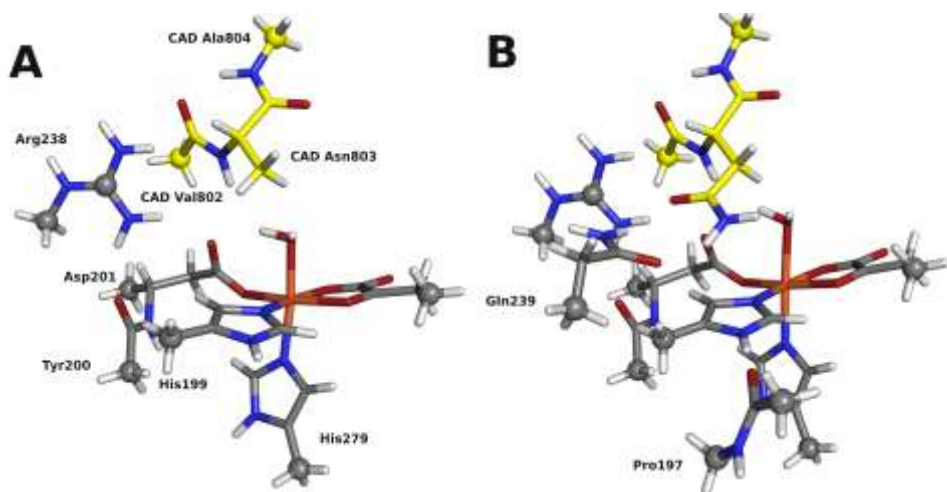


Figure S1. Models used for DFT Calculations, with frozen atoms shown as spheres. (A) The model for N803A. (B) The model for the “wild-type” approximation. C atoms of the CAD fragment are colored in yellow.

Thermodynamic Parameters

N803	ΔE	ΔH	ΔG
6C → 5C + H ₂ O CAD +	□□□□	10.5	□□□□
6C → 5C + H ₂ O CAD –	□□□□	13.8	□□□□
Difference	-5□2	-3.3	-□□□□
N803G	ΔE	ΔH	ΔG
6C → 5C + H ₂ O CAD +	12.6	11.7	-4.6
6C → 5C + H ₂ O CAD –	15.8	14.6	-0.8
Difference	-3.2	-2.9	-3.8
N803A	ΔE	ΔH	ΔG
6C → 5C + H ₂ O CAD +	11.8	11.6	-4.7
6C → 5C + H ₂ O CAD –	15.7	14.6	0.8
Difference	-3.9	-3.0	-5.5
N803A*	ΔE	ΔH	ΔG
6C → 5C + H ₂ O CAD +	9.3	9.1	-8.5
6C → 5C + H ₂ O CAD –	15.7	14.6	0.8
Difference	-6.4	-5.5	-9.3

Table S1. Changes in energy (without zero-point correction), enthalpy, and Gibbs free energy upon water dissociation for the various models. “CAD +” and “CAD –” refer to models with the CAD fragment in its crystallographic location or displaced ≈40 Å away, respectively. All energies are given in kcal / mole.

	ΔE N803G	ΔE N803A	ΔE N803A*
6C CAD + $\rightarrow$ 6C CAD –	2.6	1.4	-1.2
5C CAD + $\rightarrow$ 5C CAD –	5.8	5.3	5.2
Difference	-3.2	-2.9	-6.4

Table S2. Changes in energy (without zero-point correction), enthalpy, and Gibbs free energy upon water loss for the three models. “CAD +” and “CAD –” refer to models with the CAD fragment in its crystallographic location or displaced ≈ 40 Å away, respectively. All energies are given in kcal / mole.

	E	H	G
H₂O	-76.432337339	-76.407678000	-76.429781000
N803	E	H	G
6C CAD +	-4174.550855600	-4173.468309000	-4173.653784000
6C CAD –	-4174.519584300	-4173.439976000	-4173.646483000
5C CAD +	-4098.101132700	-4097.043895000	-4097.235115000
5C CAD –	-4098.062300900	-4097.010270000	-4097.213784000
N803G	E	H	G
6C CAD +	-3469.483014590	-3468.677549000	-3468.828582000
6C CAD –	-3469.478920440	-3468.673715000	-3468.840602000
5C CAD +	-3393.030617590	-3392.251307000	-3392.406112000
5C CAD –	-3393.021471210	-3392.242813000	-3392.412102000
N803A	E	H	G
6C CAD +	-3508.795461950	-3507.961874000	-3508.113021000
6C CAD –	-3508.793292900	-3507.958186000	-3508.133443000
5C CAD +	-3432.344285940	-3431.535777000	-3431.690779000
5C CAD –	-3432.335926680	-3431.527289000	-3431.702410000
N803A*	E	H	G
6C CAD +	-3508.791062250	-3507.959742000	-3508.106843000
6C CAD –	-3508.793023010	-3507.958780000	-3508.130371000
5C CAD +	-3432.343957100	-3431.537546000	-3431.690539000
5C CAD –	-3432.335651690	-3431.527884000	-3431.699313000

Table S3. Energy (without zero-point correction), enthalpy, and Gibbs free energy for the computational models. “CAD +” and “CAD –” refer to models with the CAD fragment in its crystallographic location or displaced ≈ 40 Å away, respectively. All energies are given in Hartree.

Table S4. Optimized coordinates for N803 CAD-bound, 6C.

Fe	1.100305	-2.666026	0.17381
O	-0.091099	-2.344078	1.873761
N	1.967094	-0.63901	0.036428
N	2.676582	-3.252152	1.45157
C	0.728528	-5.081654	-1.340495
O	0.317162	-4.489251	-0.274957
O	0.406856	-6.186341	-1.78078
C	1.76626	-4.237243	-2.119313
O	2.128552	-3.165941	-1.611143
O	-0.437519	-1.614969	-0.996616
C	6.57236	3.790679	-3.503623
C	6.083589	3.366405	-2.145462
O	5.124686	2.586583	-1.997828
N	6.767614	3.896421	-1.109124
C	6.41047	3.609838	0.256199
C	1.968634	3.028353	0.721431
C	2.151525	1.598046	0.342669
N	3.150937	1.151541	-0.506632
C	1.431332	0.469034	0.669982
C	3.001136	-0.186727	-0.667944
C	1.136728	1.359735	4.557431
C	-0.288387	0.999741	4.169401
O	-1.040395	1.848784	3.649618
N	-0.655653	-0.282625	4.410584
C	-1.99794	-0.832124	4.201814
C	-2.667745	-1.102382	5.552095
C	-1.944781	-2.112772	3.34737
C	-1.264814	-1.88516	2.000784
O	-1.900673	-1.219165	1.117378
C	-4.185452	3.333495	3.676725
N	-4.784774	3.101774	2.35999
C	-4.118541	2.520148	1.340544
N	-2.937112	1.938378	1.544611
N	-4.621363	2.587924	0.084705
C	1.283702	6.965948	-0.82823
C	-0.047407	6.440058	-1.373905
C	-0.165893	4.922569	-1.282907
O	0.612555	4.176894	-1.912666
N	-1.158563	4.447997	-0.498421
C	6.104065	-2.218276	2.442056
C	4.717927	-2.715383	2.259682
N	3.838873	-2.971038	3.302909
C	3.976455	-2.921003	1.123027
C	2.627664	-3.287926	2.776543

C	-5.23257	-1.066116	0.895859
C	-5.141703	-0.422932	-0.473075
O	-6.095465	0.220188	-0.962699
N	-3.969717	-0.593047	-1.141995
C	-3.748964	-0.055597	-2.491676
C	-4.397916	-0.96402	-3.561672
O	-3.729645	-1.624685	-4.364239
C	-2.276554	0.105976	-2.841679
C	-1.590583	1.248954	-2.128837
O	-2.142261	1.858373	-1.177167
N	-0.352882	1.565965	-2.5453
N	-5.747886	-0.923158	-3.522795
C	-6.541962	-1.783771	-4.359512
C	2.293583	-4.713086	-3.432926
C	3.284243	-3.745774	-4.071749
H	7.472906	4.418587	-3.469712
H	5.774265	4.34606	-4.01955
H	6.784747	2.89767	-4.109641
H	7.225611	3.927426	0.918296
H	6.249464	2.529919	0.384293
H	5.487421	4.133031	0.55787
H	7.516298	4.554564	-1.295893
H	3.878775	1.73263	-0.960628
H	0.550212	0.388633	1.299877
H	3.635666	-0.788971	-1.3095
H	1.035121	3.145273	1.288498
H	1.912469	3.665611	-0.171372
H	2.795823	3.392548	1.354528
H	-1.431746	3.457494	-0.584794
H	-1.846218	5.088696	-0.115699
H	1.36192	8.051839	-0.984196
H	2.127884	6.482561	-1.341501
H	1.37862	6.769307	0.251002
H	-0.889741	6.926515	-0.857311
H	-0.132599	6.69412	-2.443232
H	-2.510231	1.439903	0.761691
H	-2.394015	1.977273	2.422482
H	-4.033292	2.148345	-0.630752
H	-5.623763	2.475865	-0.050501
H	-5.54711	3.716981	2.090076
H	-4.962344	3.738278	4.334648
H	-3.344926	4.04387	3.62571
H	-3.82682	2.388576	4.106848
H	1.623099	0.603307	5.188663
H	1.126413	2.321288	5.088697
H	1.733349	1.49026	3.641399

H	0.025881	-0.894852	4.851985
H	-2.552273	-0.060814	3.65047
H	-3.687108	-1.492038	5.408194
H	-2.72959	-0.181476	6.151208
H	-2.10093	-1.851245	6.128717
H	-1.408767	-2.905139	3.892074
H	-2.9782	-2.454826	3.181635
H	-5.83246	-0.420965	1.551554
H	-4.24027	-1.24611	1.331804
H	-5.762343	-2.027679	0.801499
H	-4.26261	0.919071	-2.529105
H	-1.73597	-0.833476	-2.639644
H	-2.202131	0.255995	-3.929162
H	-7.361896	-1.219869	-4.830161
H	-6.978847	-2.620815	-3.788732
H	-5.892677	-2.195018	-5.141762
H	4.067146	-2.942386	4.292615
H	-3.227976	-1.128049	-0.688741
H	0.093856	2.445366	-2.214165
H	0.018596	1.137243	-3.389279
H	-6.178887	-0.405668	-2.748175
H	4.293835	-2.830269	0.089125
H	1.74242	-3.501582	3.364898
H	6.591033	-2.114218	1.463011
H	6.721443	-2.899709	3.050601
H	6.121259	-1.230845	2.932808
H	2.730844	-5.71448	-3.268901
H	1.421204	-4.906913	-4.083084
H	3.633532	-4.135134	-5.039392
H	4.163123	-3.594467	-3.427598
H	2.822553	-2.762518	-4.244963
H	-1.057549	-1.368811	-0.228257
H	0.012566	-0.7952	-1.271107

Table S5. Optimized coordinates for N803 CAD-bound, 5C.

Fe	0.698549	-2.632895	0.438987
O	-0.422728	-2.220417	2.072875
N	1.482901	-0.813565	-0.212676
N	2.327627	-3.062702	1.715158
C	-0.458725	-4.517999	-1.411521
O	-0.73257	-3.782506	-0.384706
O	-1.184544	-5.322666	-1.991415
C	0.988109	-4.298723	-1.907256
O	1.694305	-3.522444	-1.250216
C	7.065469	2.480197	-3.671689

C	6.477331	2.284454	-2.300028
O	5.413222	1.667628	-2.115965
N	7.216959	2.828775	-1.306247
C	6.852656	2.74089	0.080869
C	2.369614	2.726205	0.513411
C	2.178765	1.313491	0.088922
N	3.013867	0.665636	-0.808408
C	1.234388	0.37736	0.443687
C	2.563281	-0.601394	-0.965855
C	1.318387	1.603273	4.491537
C	-0.139101	1.388677	4.111767
O	-0.773235	2.269369	3.496311
N	-0.666035	0.193535	4.472912
C	-2.065673	-0.208033	4.300261
C	-2.753664	-0.281442	5.670985
C	-2.163459	-1.54467	3.541006
C	-1.481882	-1.504858	2.165275
O	-1.966354	-0.785089	1.255818
C	-3.731927	4.060806	3.28646
N	-4.329922	3.777601	1.979009
C	-3.740294	2.988766	1.056107
N	-2.641687	2.296812	1.354216
N	-4.229793	2.948634	-0.207584
C	2.158192	6.517832	-1.474832
C	0.765087	6.098157	-1.954423
C	0.485529	4.615456	-1.732061
O	1.167615	3.742993	-2.306924
N	-0.533511	4.310479	-0.895733
C	5.855246	-2.732616	2.888845
C	4.403341	-2.936655	2.611867
N	3.466334	-3.230344	3.593188
C	3.669249	-2.850363	1.451109
C	2.237956	-3.294453	3.019253
C	-5.258549	-0.473853	0.986029
C	-5.05792	-0.058453	-0.448837
O	-5.902557	0.62857	-1.067424
N	-3.915961	-0.506759	-1.022044
C	-3.543906	-0.197022	-2.404126
C	-4.30489	-1.092605	-3.428
O	-3.724298	-1.868053	-4.194485
C	-2.029588	-0.29959	-2.589263
C	-1.317271	0.983909	-2.196533
O	-1.812067	1.76509	-1.342012
N	-0.149852	1.242176	-2.797571
N	-5.642593	-0.876201	-3.393803
C	-6.598801	-1.620975	-4.184722

C	1.493241	-5.009743	-3.118931
C	2.931313	-4.647486	-3.475005
H	7.987982	3.07643	-3.676598
H	6.323154	2.970853	-4.318703
H	7.279012	1.497325	-4.118718
H	7.651	2.264098	0.671058
H	5.944725	2.130482	0.151877
H	6.648235	3.735755	0.508344
H	8.071749	3.317245	-1.55131
H	3.848272	1.070955	-1.263542
H	0.379498	0.485826	1.103888
H	3.029317	-1.335876	-1.614653
H	1.492177	3.065398	1.080356
H	2.493288	3.384596	-0.357347
H	3.256408	2.842887	1.159729
H	-0.917629	3.351878	-0.910638
H	-1.148359	5.048905	-0.568764
H	2.349859	7.572356	-1.721816
H	2.932144	5.904429	-1.959212
H	2.257327	6.400011	-0.384507
H	-0.007376	6.716702	-1.470236
H	0.682657	6.26851	-3.04043
H	-2.297156	1.611154	0.676942
H	-2.099047	2.386785	2.228588
H	-3.689917	2.360205	-0.850244
H	-5.238194	2.914465	-0.341478
H	-4.992699	4.457405	1.616743
H	-4.459786	4.627749	3.877423
H	-2.802427	4.644615	3.194221
H	-3.510077	3.124216	3.815296
H	1.694786	0.866896	5.21534
H	1.429225	2.612131	4.911787
H	1.935692	1.550738	3.581617
H	-0.066237	-0.449992	4.983166
H	-2.527034	0.577973	3.687543
H	-3.813497	-0.556908	5.558253
H	-2.698182	0.6881 6	.188213
H	-2.275736	-1.041791	6.309829
H	-1.720191	-2.350672	4.146326
H	-3.231412	-1.779647	3.404051
H	-5.875656	0.276492	1.497736
H	-4.297595	-0.604055	1.503485
H	-5.804662	-1.430872	1.01058
H	-3.871299	0.838662	-2.602195
H	-1.621601	-1.119996	-1.972608
H	-1.819605	-0.57378	-3.633

H	-7.223048	-0.941695	-4.786366
H	-7.25841	-2.229015	-3.544496
H	-6.044461	-2.287064	-4.857834
H	3.665946	-3.386341	4.577251
H	-3.21277	-0.937643	-0.410872
H	0.391933	2.096047	-2.560959
H	0.223509	0.604364	-3.493389
H	-5.984389	-0.213049	-2.686436
H	4.021435	-2.635084	0.447824
H	1.316545	-3.480341	3.55993
H	6.385856	-2.530414	1.94884
H	6.316761	-3.620105	3.351412
H	6.025071	-1.878179	3.564301
H	1.368336	-6.092554	-2.935366
H	0.788893	-4.798264	-3.943612
H	3.257773	-5.201465	-4.367197
H	3.617092	-4.89002	-2.650115
H	3.028835	-3.572163	-3.6866

Table S6. Optimized coordinates for N803 CAD-unbound, 6C.

Fe	-16.004101	-0.88637	2.332517
O	-16.046764	-2.470027	1.001615
N	-15.454768	0.660772	0.978826
N	-18.110202	-0.285164	2.075844
C	-16.460548	-1.347947	5.150763
O	-16.505427	-1.948247	4.00909
O	-16.714548	-1.807147	6.267238
C	-16.034715	0.127463	5.018799
O	-15.784491	0.54576	3.878066
O	-13.842716	-1.31801	2.396997
C	-15.24777	7.781909	-0.502749
C	-15.915734	6.512329	-0.907173
O	-15.646446	5.411232	-0.396837
N	-16.828746	6.678123	-1.884408
C	-17.4963	5.552792	-2.455273
C	-15.029915	1.85584	-2.510169
C	-15.211379	1.588914	-1.061455
N	-15.456054	2.5759	-0.120295
C	-15.21152	0.407184	-0.356912
C	-15.59173	1.979242	1.08928
C	-17.449057	-1.519869	-3.405051
C	-16.356324	-2.465434	-2.923016
O	-15.176144	-2.359773	-3.319594
N	-16.770235	-3.42055	-2.056046
C	-15.962498	-4.557098	-1.616845

C	-16.679195	-5.849317	-2.018332
C	-15.678228	-4.534443	-0.100812
C	-15.178496	-3.183085	0.409519
O	-13.963052	-2.85176	0.212917
C	-12.743863	-4.190587	-4.876365
N	-11.455236	-3.942178	-4.238709
C	-11.35835	-3.558957	-2.957926
N	-12.462102	-3.154884	-2.310922
N	-10.157209	-3.554315	-2.341911
C	-12.031854	3.749752	-4.945993
C	-11.123112	2.707708	-4.285973
C	-11.802742	2.095478	-3.065881
O	-12.112117	2.779163	-2.084982
N	-12.040641	0.754629	-3.129929
C	-20.995353	1.80251	0.902973
C	-19.978772	0.877456	1.499398
N	-20.237365	0.047101	2.579927
C	-18.652515	0.642722	1.201766
C	-19.098276	-0.628318	2.893325
C	-15.925096	1.002765	6.226514
C	-15.576829	2.45004	5.889452
C	56.140606	-2.79859	-0.666663
C	57.291304	-1.832904	-0.471927
O	58.467426	-2.165318	-0.701966
N	56.964438	-0.594791	-0.012588
C	57.958544	0.457607	0.216716
C	58.64062	0.282086	1.599467
O	58.51839	1.110856	2.509649
C	57.318861	1.834781	0.082015
C	57.013732	2.179414	-1.377077
O	57.695238	1.759341	-2.314222
N	55.934137	2.99438	-1.560352
N	59.362606	-0.864089	1.68509
C	59.990915	-1.311662	2.91281
H	-15.74487	8.681758	-0.889866
H	-14.206031	7.778057	-0.861803
H	-15.203227	7.846859	0.594061
H	-16.948032	7.594066	-2.302885
H	-18.421525	5.878742	-2.94906
H	-17.752533	4.837845	-1.661625
H	-16.871149	5.027642	-3.198649
H	-14.731664	0.936274	-3.029036
H	-14.262161	2.621504	-2.675519
H	-15.968856	2.207731	-2.973271
H	-15.039815	-0.602604	-0.717566
H	-15.795883	2.511814	2.012124

H	-15.524854	3.592015	-0.301041
H	-18.450929	-1.794734	-3.049563
H	-17.447396	-1.513666	-4.504672
H	-17.219402	-0.497995	-3.068566
H	-17.745218	-3.410614	-1.766619
H	-16.095992	-6.730486	-1.709364
H	-16.82881	-5.895481	-3.10746
H	-17.664843	-5.916178	-1.529615
H	-15.012689	-4.466736	-2.161071
H	-16.597872	-4.787891	0.447411
H	-14.925369	-5.309091	0.114176
H	-10.096675	-3.236891	-1.379821
H	-9.425046	-4.184928	-2.653235
H	-12.56244	-3.140855	-1.287881
H	-13.352135	-2.970214	-2.799585
H	-10.604	-4.048572	-4.781474
H	-12.553338	-4.626903	-5.86325
H	-13.328175	-3.26745	-5.00725
H	-13.332109	-4.905806	-4.283882
H	-10.825909	1.936068	-5.01449
H	-10.200749	3.192765	-3.928316
H	-11.512775	4.253731	-5.774807
H	-12.330519	4.51072	-4.210565
H	-12.945019	3.284757	-5.34981
H	-12.466776	0.289025	-2.333626
H	-11.764457	0.192085	-3.926225
H	-20.550121	2.345729	0.05845
H	-21.347578	2.546836	1.635673
H	-21.878103	1.258963	0.528466
H	-18.055899	1.090671	0.413458
H	-19.026251	-1.35104	3.699585
H	-21.12638	-0.044006	3.063412
H	-16.873453	0.918608	6.786163
H	-15.176442	0.543176	6.898069
H	-15.496408	3.051307	6.807132
H	-16.347989	2.904096	5.249317
H	-14.618924	2.512662	5.35282
H	-13.693306	-1.826483	1.54356
H	-13.294943	-0.516687	2.367333
H	55.775139	3.377011	-2.488395
H	55.469874	3.447407	-0.77994
H	58.714211	0.341139	-0.576361
H	56.422195	1.918117	0.717618
H	58.029109	2.581471	0.472091
H	59.357147	-1.475643	0.860269
H	61.063282	-1.506225	2.755943

H	59.519108	-2.233236	3.291697
H	59.876296	-0.51702	3.660422
H	56.201429	-3.220309	-1.680057
H	55.150842	-2.341387	-0.528591
H	56.250809	-3.632948	0.042358
H	56.00065	-0.404725	0.249068

Table S7. Optimized coordinates for N803 CAD-unbound, 5C.

Fe	-16.361705	-0.698814	2.372371
O	-16.336633	-2.403283	1.336015
N	-15.613168	0.679191	1.014809
N	-18.393376	-0.110115	2.170124
C	-16.453265	-0.983503	5.264328
O	-16.557853	-1.644464	4.161814
O	-16.548064	-1.399931	6.421189
C	-16.184246	0.51611	5.016168
O	-16.103604	0.887871	3.838569
C	-15.555325	7.679371	-1.082893
C	-16.221704	6.376436	-1.373333
O	-15.934015	5.317536	-0.789709
N	-17.154699	6.462504	-2.343216
C	-17.808178	5.290215	-2.830426
C	-15.341293	1.602095	-2.571963
C	-15.454201	1.445518	-1.099559
N	-15.681147	2.501581	-0.229702
C	-15.40952	0.322506	-0.306947
C	-15.767258	2.003943	1.025984
C	-17.762246	-1.838074	-3.166379
C	-16.665718	-2.751855	-2.635366
O	-15.497875	-2.695051	-3.072684
N	-17.067376	-3.6177	-1.673628
C	-16.259467	-4.711806	-1.135744
C	-16.988414	-6.031672	-1.412946
C	-15.958099	-4.530402	0.367571
C	-15.470435	-3.11407	0.70628
O	-14.333104	-2.730013	0.339946
C	-13.060198	-4.626097	-4.412962
N	-11.767393	-4.361254	-3.788391
C	-11.670126	-3.831364	-2.559466
N	-12.77187	-3.336965	-1.978371
N	-10.472135	-3.77316	-1.938684
C	-12.349485	3.278619	-5.169307
C	-11.444304	2.285389	-4.431947
C	-12.115664	1.792752	-3.154018
O	-12.421081	2.571692	-2.245563

N	-12.375008	0.45519	-3.090209
C	-21.298699	1.843978	0.847394
C	-20.26703	0.991499	1.516281
N	-20.500119	0.288291	2.6892
C	-18.951003	0.717879	1.210551
C	-19.358105	-0.353999	3.048958
C	-16.035809	1.460852	6.16621
C	-15.868266	2.919066	5.746399
C	55.833988	-2.880467	-0.50425
C	56.954139	-1.868184	-0.379014
O	58.137269	-2.17327	-0.61097
N	56.591985	-0.618684	0.019491
C	57.554164	0.474947	0.184633
C	58.260555	0.386723	1.563474
O	58.118641	1.25002	2.438125
C	56.869754	1.824226	-0.002141
C	56.544446	2.101049	-1.471104
O	57.227309	1.658385	-2.396783
N	55.4453	2.883945	-1.676811
N	59.028231	-0.725441	1.688458
C	59.692625	-1.090435	2.924325
H	-16.099754	8.547236	-1.479231
H	-14.542633	7.676856	-1.517506
H	-15.433927	7.803316	0.002695
H	-17.286259	7.342897	-2.829133
H	-18.739601	5.56772	-3.341824
H	-18.051975	4.629334	-1.987443
H	-17.177986	4.722066	-3.537019
H	-15.045336	0.649989	-3.029491
H	-14.596697	2.365163	-2.830392
H	-16.306451	1.901614	-3.017241
H	-15.216909	-0.710768	-0.581594
H	-15.953065	2.603647	1.910493
H	-15.767267	3.497968	-0.490662
H	-18.762214	-2.091528	-2.789478
H	-17.766818	-1.893642	-4.26436
H	-17.532325	-0.798236	-2.889245
H	-18.037945	-3.574986	-1.373274
H	-16.408765	-6.885896	-1.030149
H	-17.147376	-6.174203	-2.492336
H	-17.970116	-6.046887	-0.911877
H	-15.314866	-4.67712	-1.695196
H	-16.862801	-4.745388	0.955794
H	-15.18543	-5.263464	0.651137
H	-10.418789	-3.358266	-1.013692
H	-9.749035	-4.446788	-2.171328

H	-12.901263	-3.200424	-0.965535
H	-13.656934	-3.217176	-2.494439
H	-10.916487	-4.541749	-4.311415
H	-12.87873	-5.168165	-5.347831
H	-13.608055	-3.700331	-4.643686
H	-13.680046	-5.253897	-3.757082
H	-11.168861	1.448662	-5.094657
H	-10.510206	2.786505	-4.131146
H	-11.837365	3.696976	-6.048587
H	-12.624486	4.107274	-4.500962
H	-13.27557	2.792588	-5.514462
H	-12.746482	0.072374	-2.224643
H	-12.023935	-0.193942	-3.784846
H	-20.882202	2.278522	-0.071315
H	-21.623821	2.673335	1.496322
H	-22.194611	1.26441	0.57162
H	-18.370678	1.073034	0.364249
H	-19.267122	-0.98237	3.929115
H	-21.377518	0.260094	3.201383
H	-16.907698	1.310874	6.827387
H	-15.18156	1.10277	6.770237
H	-15.757138	3.562803	6.631206
H	-16.740562	3.269746	5.174887
H	-14.978757	3.049476	5.112931
H	55.270489	3.225887	-2.617818
H	54.980529	3.360148	-0.910599
H	58.302808	0.346173	-0.613146
H	55.975477	1.906185	0.637001
H	57.558781	2.607971	0.351836
H	59.033527	-1.374557	0.892789
H	60.769554	-1.248907	2.758331
H	59.264579	-2.011777	3.352521
H	59.556844	-0.267449	3.636843
H	55.885914	-3.343329	-1.500098
H	54.832169	-2.451766	-0.361379
H	55.99009	-3.679036	0.236553
H	55.625798	-0.447484	0.285296

Table S8. Optimized coordinates for model N803G CAD-bound, 6C.

Fe	2.030799	0.627908	-0.417164
N	1.701033	-0.204289	1.557417
O	0.856987	-0.708390	-1.472777
N	3.831336	-0.533388	-0.587456
C	3.226269	2.877064	-1.759575
O	2.548072	1.803998	-1.995508

O	3.623380	3.723584	-2.561396
C	3.553699	3.043096	-0.260649
O	3.105654	2.187552	0.518588
C	0.477103	-2.788581	3.949158
C	1.082612	-1.682120	3.155191
N	2.026695	-0.795779	3.653440
C	0.895250	-1.290198	1.848473
C	2.370905	0.073780	2.669173
C	0.404276	-5.113812	0.374303
C	-0.700664	-4.242371	-0.189111
O	-1.688326	-3.928358	0.507525
N	-0.515044	-3.831308	-1.465664
C	-1.481883	-3.074514	-2.260559
C	-1.919849	-3.917229	-3.458744
C	-0.896461	-1.724158	-2.712477
C	-0.392531	-0.875859	-1.550141
O	-1.245798	-0.402516	-0.718897
C	-5.221433	-3.952980	0.361806
N	-5.584016	-2.654643	0.923579
C	-4.753992	-1.598467	0.963357
N	-3.476564	-1.733034	0.605841
N	-5.231035	-0.418256	1.426844
C	6.485628	-2.892721	0.561254
C	5.557274	-1.907629	-0.064507
N	5.876916	-1.129778	-1.166036
C	4.278100	-1.523644	0.268360
C	4.819825	-0.321395	-1.447821
C	-4.141696	0.683185	-1.989067
C	-4.396085	1.530645	-0.764084
O	-5.536008	1.901245	-0.427409
N	-3.291271	1.832015	-0.019212
C	-3.332233	2.704558	1.154742
C	-3.437968	4.204938	0.814801
O	-2.536929	5.000878	1.092192
N	-4.610015	4.517494	0.207055
C	-4.892765	5.831911	-0.323341
C	4.382397	4.190176	0.216225
C	4.768846	4.071384	1.686847
H	0.213489	-1.703175	1.112146
H	3.097896	0.871191	2.783620
H	2.396292	-0.790837	4.600326
H	-0.241604	-3.335264	3.323100
H	-0.060859	-2.413347	4.835067
H	1.237120	-3.504674	4.301578
H	1.077842	-5.515721	-0.394707
H	-0.047999	-5.946421	0.930075

H	1.001350	-4.523789	1.086725
H	-2.663765	-3.376670	-4.063910
H	-2.364913	-4.867303	-3.127768
H	-2.337030	-2.890250	-1.597166
H	-0.063472	-1.892060	-3.410998
H	-1.682799	-1.170739	-3.250801
H	0.325499	-4.145914	-1.945412
H	-1.062182	-4.146445	-4.111672
H	-2.887342	-0.937987	0.340107
H	-2.996846	-2.647404	0.525893
H	-4.574935	0.356447	1.447179
H	-6.180835	-0.146577	1.184462
H	-6.453823	-2.580341	1.442887
H	-6.131237	-4.559347	0.294272
H	-4.484327	-4.481490	0.985603
H	-4.809468	-3.823815	-0.648905
H	5.987035	-3.385455	1.406992
H	7.399242	-2.408746	0.943806
H	6.798214	-3.676147	-0.148366
H	3.656344	-1.902745	1.072866
H	4.798681	0.383227	-2.272621
H	6.752322	-1.155886	-1.681546
H	-3.188630	0.142122	-1.929720
H	-4.123924	1.336595	-2.876453
H	-4.976708	-0.018535	-2.117022
H	-2.374974	1.619111	-0.414354
H	-4.195446	2.422089	1.779644
H	-5.827761	6.234797	0.096696
H	-4.983654	5.808172	-1.421390
H	-4.063573	6.495421	-0.048269
H	-5.250101	3.743143	0.004903
H	5.373528	4.935895	1.997938
H	5.357925	3.159708	1.867878
H	3.877034	4.028833	2.328804
H	5.259966	4.268049	-0.448418
H	3.808986	5.114373	0.014072
H	-2.414425	2.551854	1.732339
O	0.129934	1.686695	0.052734
H	-0.469678	0.881662	-0.035737
H	0.133046	1.977677	0.979750

Table S9. Optimized coordinates for model N803G CAD-bound, 5C.

Fe	1.998719	0.588387	-0.385366
N	1.538266	-0.027138	1.559258
O	0.873185	-0.670877	-1.481062

N	3.818761	-0.469333	-0.546824
C	2.906027	3.001168	-1.687989
O	2.251662	1.904656	-1.888277
O	3.169798	3.891420	-2.494856
C	3.393420	3.126527	-0.226343
O	3.073082	2.218999	0.551876
C	0.607346	-2.738548	3.936208
C	1.073150	-1.563127	3.149981
N	1.923061	-0.586781	3.651881
C	0.841873	-1.188560	1.846770
C	2.179873	0.314820	2.673453
C	0.518284	-5.070573	0.366124
C	-0.606326	-4.213175	-0.184161
O	-1.592524	-3.922761	0.524973
N	-0.442355	-3.789525	-1.459640
C	-1.434995	-3.051574	-2.243204
C	-1.866603	-3.908091	-3.439937
C	-0.891262	-1.681330	-2.694767
C	-0.395043	-0.807181	-1.536407
O	-1.220211	-0.307652	-0.719333
C	-5.120495	-3.976358	0.420839
N	-5.492142	-2.681495	0.986312
C	-4.673661	-1.615473	1.012956
N	-3.396936	-1.740515	0.646764
N	-5.158281	-0.434291	1.466361
C	6.574698	-2.777439	0.474999
C	5.585493	-1.820363	-0.105389
N	5.786450	-1.130631	-1.290857
C	4.350664	-1.395219	0.333355
C	4.711050	-0.332245	-1.520410
C	-4.124648	0.668241	-1.950413
C	-4.304588	1.531276	-0.725293
O	-5.424718	1.937918	-0.356355
N	-3.162291	1.824913	-0.044727
C	-3.128013	2.741990	1.096164
C	-3.294030	4.229409	0.703556
O	-2.369183	5.038586	0.820113
N	-4.543679	4.519459	0.257190
C	-4.916168	5.810545	-0.283598
C	4.225913	4.292949	0.196760
C	4.789496	4.167804	1.610551
H	0.202735	-1.660489	1.108458
H	2.829056	1.176596	2.785431
H	2.287539	-0.546276	4.600144
H	-0.091548	-3.329991	3.328823
H	0.083452	-2.437246	4.857913

H	1.444200	-3.393170	4.229499
H	1.196851	-5.451053	-0.409420
H	0.082352	-5.917790	0.912833
H	1.106283	-4.478546	1.084142
H	-2.631946	-3.386430	-4.034858
H	-2.281971	-4.869256	-3.102581
H	-2.288260	-2.893101	-1.570430
H	-0.063786	-1.829019	-3.404816
H	-1.700409	-1.154612	-3.226177
H	0.400005	-4.082418	-1.949601
H	-1.010625	-4.113518	-4.102947
H	-2.812217	-0.944945	0.366049
H	-2.913328	-2.652543	0.567906
H	-4.512820	0.349979	1.475627
H	-6.113984	-0.176031	1.233740
H	-6.359899	-2.614608	1.509919
H	-6.023125	-4.594944	0.369175
H	-4.366668	-4.493855	1.033687
H	-4.726432	-3.843528	-0.596537
H	6.176960	-3.202158	1.406540
H	7.530947	-2.282854	0.710704
H	6.791061	-3.611650	-0.211792
H	3.817861	-1.699031	1.229300
H	4.608476	0.312060	-2.387662
H	6.601459	-1.207507	-1.893156
H	-3.187922	0.096664	-1.917817
H	-4.109170	1.319002	-2.839845
H	-4.986833	-0.004452	-2.050794
H	-2.281010	1.419604	-0.377496
H	-3.926684	2.472818	1.808687
H	-5.823580	6.192895	0.208871
H	-5.103376	5.751936	-1.368330
H	-4.089107	6.508398	-0.102485
H	-5.176402	3.722391	0.127313
H	5.401259	5.047606	1.857328
H	5.421884	3.272576	1.706873
H	3.982947	4.093099	2.354564
H	5.016771	4.421982	-0.562501
H	3.597746	5.196196	0.081470
H	-2.158861	2.631362	1.594287

Table S10. Optimized coordinates for model N803G CAD-unbound, 6C.

Fe	9.225343	1.637372	-0.368040
N	9.374038	0.857046	1.610590
O	8.667560	-0.111289	-1.297447

N	11.411930	1.343676	-0.585148
C	9.570153	4.113824	-1.791697
O	9.282260	2.871563	-1.989416
O	9.693190	5.011546	-2.627653
C	9.771282	4.442743	-0.296697
O	9.612043	3.523294	0.520178
C	9.719032	-2.020409	3.926978
C	9.647491	-0.745271	3.172296
N	10.067113	0.481912	3.664476
C	9.214570	-0.483248	1.894804
C	9.886598	1.418900	2.697513
C	10.583994	-4.093354	0.320996
C	9.177725	-3.811588	-0.193215
O	8.169264	-4.014380	0.515283
N	9.116479	-3.330175	-1.458876
C	7.888356	-3.199731	-2.241945
C	8.043033	-4.015279	-3.525713
C	7.526153	-1.737966	-2.579828
C	7.595420	-0.788569	-1.387463
O	6.618648	-0.729906	-0.572120
C	5.274736	-5.894816	0.374331
N	4.179668	-5.104840	0.926041
C	4.178534	-3.764549	0.883676
N	5.301096	-3.121650	0.536498
N	3.058307	-3.081698	1.200316
C	14.967473	0.697172	0.418775
C	13.623909	1.012235	-0.164881
N	13.447199	1.579075	-1.418119
C	12.342289	0.871101	0.326204
C	12.115711	1.762310	-1.630477
C	10.139399	5.826376	0.117223
C	10.302816	6.024574	1.622404
H	9.302850	-2.831248	3.313070
H	9.144651	-1.981310	4.867384
H	10.756319	-2.289351	4.186772
H	8.784761	-1.168913	1.172253
H	10.138532	2.468645	2.805256
H	10.442766	0.655603	4.592884
H	11.342475	-4.094456	-0.473128
H	10.584582	-5.070182	0.823975
H	10.860031	-3.333606	1.068207
H	7.096102	-3.629159	-1.613767
H	7.131345	-3.950534	-4.139249
H	8.236338	-5.075132	-3.301658
H	8.213993	-1.363498	-3.352832
H	6.506238	-1.733568	-2.995125

H	8.878339	-3.631263	-4.133882
H	9.993685	-3.176333	-1.950125
H	5.339741	-2.146307	0.216783
H	6.221996	-3.585808	0.528537
H	3.077156	-2.067053	1.202646
H	2.148322	-3.520455	1.099865
H	3.418399	-5.576319	1.403497
H	4.978934	-6.949497	0.401485
H	6.205436	-5.775306	0.949615
H	5.459308	-5.607982	-0.671005
H	14.842711	0.240174	1.409802
H	15.582313	1.603930	0.539353
H	15.533400	-0.008820	-0.210487
H	12.038245	0.458574	1.283057
H	11.700429	2.190898	-2.536712
H	14.185477	1.826416	-2.070981
H	11.059023	6.094760	-0.434675
H	9.377139	6.505923	-0.305883
H	10.577050	7.066436	1.842866
H	11.089884	5.370159	2.026434
H	9.368829	5.795692	2.157022
H	-39.309436	0.270806	0.206296
H	-39.675652	3.243956	0.011576
H	-40.256288	2.117941	-1.255500
H	-41.051675	2.148549	0.346501
C	-40.085558	2.243299	-0.173679
N	-39.129780	1.273631	0.323897
H	-36.100726	0.767827	1.604936
H	-35.796308	-0.118884	-0.545837
O	-37.511993	2.782392	0.963332
C	-37.905879	1.622213	0.802004
C	-37.016547	0.402641	1.126469
N	-36.654840	-0.364063	-0.062076
H	-37.168513	-3.016727	-1.813825
H	-37.626186	-1.579945	-2.744275
H	-35.955996	-1.735566	-2.123422
O	-38.620188	-1.514681	-0.147989
C	-37.501663	-1.264785	-0.630765
C	-37.014001	-1.932012	-1.899924
H	-37.542188	-0.273440	1.818138
O	7.082667	1.810965	0.048637
H	6.836083	2.148352	0.924536
H	6.754958	0.863057	-0.031317

Table S11. Optimized coordinates for model N803G CAD-unbound, 5C.

Fe	9.525971	1.610477	-0.387290
N	9.495010	0.919510	1.587645
O	8.829436	0.044370	-1.315403
N	11.624409	1.390202	-0.591302
C	9.661584	4.188988	-1.767539
O	9.436812	2.942214	-1.957547
O	9.701857	5.108936	-2.588487
C	9.913942	4.522944	-0.267977
O	9.760901	3.622115	0.561805
C	9.928408	-1.940315	3.931050
C	9.797556	-0.669371	3.168443
N	10.124405	0.579889	3.673790
C	9.400399	-0.430678	1.873635
C	9.927983	1.506670	2.697834
C	10.796636	-4.016632	0.327737
C	9.388346	-3.760315	-0.194256
O	8.381077	-3.999913	0.501872
N	9.328106	-3.251917	-1.450710
C	8.102975	-3.118390	-2.240674
C	8.255785	-3.947083	-3.519222
C	7.760451	-1.649998	-2.569569
C	7.800456	-0.735090	-1.341245
O	6.913564	-0.792899	-0.463264
C	5.489943	-5.825633	0.382978
N	4.378434	-5.038771	0.908112
C	4.390647	-3.696282	0.889610
N	5.524474	-3.063878	0.568022
N	3.273353	-3.006993	1.203692
C	15.173206	0.780416	0.419751
C	13.830660	1.077333	-0.166562
N	13.648680	1.598550	-1.440600
C	12.554313	0.953004	0.336526
C	12.320350	1.772706	-1.656458
C	10.337721	5.902251	0.111348
C	10.542527	6.128860	1.606636
H	9.550857	-2.772551	3.320821
H	9.351004	-1.923129	4.870026
H	10.977293	-2.157385	4.192613
H	9.021896	-1.135675	1.141455
H	10.117002	2.568081	2.816767
H	10.440234	0.777944	4.619152
H	11.559288	-4.009457	-0.462638
H	10.811350	-4.990301	0.836267
H	11.056808	-3.248124	1.071815
H	7.305825	-3.536864	-1.611387
H	7.345164	-3.883864	-4.134661

H	8.443376	-5.005325	-3.283306
H	8.464244	-1.266694	-3.323406
H	6.748721	-1.630047	-3.005779
H	9.094284	-3.573704	-4.129677
H	10.206541	-3.084946	-1.935571
H	5.593932	-2.087532	0.251474
H	6.435312	-3.545954	0.552249
H	3.304520	-1.992680	1.218207
H	2.360561	-3.433924	1.081252
H	3.617921	-5.511334	1.385763
H	5.186544	-6.878648	0.378608
H	6.400273	-5.723157	0.993163
H	5.713606	-5.520261	-0.649104
H	15.052547	0.362063	1.428064
H	15.792428	1.688355	0.502535
H	15.732941	0.048859	-0.185372
H	12.250945	0.579117	1.309486
H	11.897956	2.172878	-2.572502
H	14.386616	1.822024	-2.103008
H	11.252174	6.118163	-0.471853
H	9.591403	6.593171	-0.319948
H	10.857299	7.165288	1.795394
H	11.315697	5.457106	2.008522
H	9.613485	5.945549	2.166482
H	-39.103140	0.275362	0.204492
H	-39.473555	3.247711	0.005575
H	-40.052500	2.119027	-1.259893
H	-40.848053	2.150851	0.342001
C	-39.882031	2.246201	-0.178243
N	-38.924943	1.278589	0.320821
H	-35.895208	0.778732	1.602576
H	-35.589409	-0.110069	-0.547196
O	-37.309192	2.790476	0.958007
C	-37.701489	1.629531	0.798352
C	-36.810454	0.411639	1.124466
N	-36.447539	-0.356005	-0.063103
H	-36.956046	-3.011796	-1.810928
H	-37.417763	-1.577781	-2.743616
H	-35.746884	-1.728165	-2.123285
O	-38.411178	-1.509646	-0.147635
C	-37.293035	-1.258650	-0.630723
C	-36.804294	-1.926838	-1.898956
H	-37.335197	-0.264356	1.816898

Table S12. Optimized coordinates for model N803G CAD-unbound, FIH R238 Unbound, 5C.

Fe	11.883638	-3.663923	0.099935
N	11.533457	-2.369752	-1.542055
O	12.091703	-2.489726	1.840656
N	14.005879	-3.479849	-0.032228
C	12.383824	-6.555391	0.370623
O	11.938243	-5.515629	0.970696
O	12.628726	-7.672046	0.836908
C	12.625085	-6.327845	-1.154980
O	12.226379	-5.281815	-1.659553
C	11.302142	1.018872	-3.108593
C	11.439590	-0.401964	-2.667094
N	11.965748	-1.397879	-3.476557
C	11.163786	-1.035716	-1.472709
C	12.004443	-2.558254	-2.770949
C	12.003705	2.016785	0.960821
C	10.822573	1.189638	1.433638
O	9.736735	1.218374	0.836025
N	11.051587	0.422850	2.535587
C	10.005674	-0.331616	3.219129
C	9.759464	0.290277	4.599997
C	10.345463	-1.834543	3.348662
C	10.830601	-2.470709	2.053696
O	10.024508	-2.962905	1.209740
C	-12.846883	36.761172	0.604717
N	-13.865204	35.849578	0.112829
C	-13.574283	34.721169	-0.539071
N	-12.302396	34.426210	-0.846059
N	-14.559706	33.871398	-0.876043
C	17.157638	-1.596807	-0.636644
C	16.015307	-2.468345	-0.255631
N	16.072134	-3.436586	0.735441
C	14.721444	-2.520458	-0.717757
C	14.846976	-4.014773	0.841643
C	13.351004	-7.388522	-1.931950
C	13.513199	-7.090904	-3.420028
H	10.809139	1.599814	-2.317066
H	10.692702	1.109775	-4.022531
H	12.282418	1.480340	-3.313031
H	10.695462	-0.617258	-0.586341
H	12.374287	-3.500288	-3.161173
H	12.255524	-1.287240	-4.444070
H	12.852835	2.021789	1.659647
H	11.666791	3.050326	0.797855

H	12.352249	1.625586	-0.007356
H	9.116351	-0.216629	2.582870
H	8.967803	-0.252515	5.140383
H	9.453241	1.342683	4.503005
H	11.135195	-1.964601	4.106159
H	9.443545	-2.358221	3.700190
H	10.674164	0.249746	5.214493
H	11.979105	0.430484	2.951009
H	-12.058246	33.531637	-1.257844
H	-11.577958	35.135738	-0.822340
H	-14.376789	33.050609	-1.443134
H	-15.479411	33.946447	-0.454087
H	-14.841038	36.122503	0.178958
H	-12.357570	37.313695	-0.213931
H	-12.092268	36.213506	1.187585
H	-13.327127	37.488240	1.268441
H	16.847295	-0.908752	-1.434848
H	18.018830	-2.176254	-1.009242
H	17.511955	-0.988019	0.211715
H	14.262862	-1.914349	-1.492773
H	14.601552	-4.785258	1.565317
H	16.886045	-3.667709	1.298250
H	14.326008	-7.527155	-1.429125
H	12.823612	-8.340467	-1.747956
H	14.057599	-7.906886	-3.917544
H	14.073434	-6.157312	-3.579606
H	12.534756	-6.982072	-3.911110
H	-36.337925	-11.510787	-0.030629
H	-36.051381	-14.329529	-1.025444
H	-36.533447	-13.961336	0.659906
H	-37.650001	-13.596180	-0.689222
C	-36.591538	-13.619590	-0.386831
N	-35.978016	-12.316771	-0.553054
H	-33.423687	-10.591742	-1.806836
H	-32.915321	-10.477516	0.478651
O	-34.225829	-13.002440	-1.880825
C	-34.820551	-12.128595	-1.240745
C	-34.290014	-10.681987	-1.141634
N	-33.883466	-10.322852	0.213941
H	-34.599256	-8.701836	2.897129
H	-34.578122	-10.439811	3.240487
H	-33.116025	-9.652170	2.576172
O	-35.997083	-9.858136	0.929124
C	-34.779691	-9.949063	1.167211
C	-34.214441	-9.669003	2.544023
H	-35.068047	-9.971847	-1.461351

Table S13. Optimized coordinates for model N803A CAD-bound, 6C.

Fe	2.090317	0.632443	-0.463349
N	1.740928	-0.159569	1.535939
O	0.954566	-0.768030	-1.481815
N	3.913680	-0.486225	-0.582585
C	3.288837	2.862361	-1.838222
O	2.629283	1.775752	-2.062684
O	3.702628	3.688754	-2.652630
C	3.566522	3.079739	-0.335332
O	3.111803	2.239412	0.456350
C	0.552283	-2.717369	3.978072
C	1.138866	-1.614359	3.163111
N	2.055347	-0.693201	3.650081
C	0.957900	-1.257536	1.844957
C	2.389872	0.160865	2.648886
C	0.613394	-5.128250	0.460170
C	-0.510601	-4.306466	-0.141077
O	-1.520642	-4.009829	0.530912
N	-0.315965	-3.917138	-1.423177
C	-1.294249	-3.213414	-2.252202
C	-1.680143	-4.096781	-3.438641
C	-0.749443	-1.854340	-2.727759
C	-0.289694	-0.960347	-1.581678
O	-1.170026	-0.474483	-0.785878
C	-5.044596	-4.145375	0.326416
N	-5.451490	-2.850460	0.862398
C	-4.660866	-1.763782	0.878352
N	-3.376491	-1.861438	0.533317
N	-5.187310	-0.592448	1.306991
C	6.618781	-2.713276	0.693500
C	5.672313	-1.784149	0.015028
N	5.985935	-1.036462	-1.108506
C	4.376760	-1.430622	0.314542
C	4.908628	-0.272908	-1.435302
C	-4.068896	0.465139	-2.118527
C	-4.428459	1.328819	-0.927959
O	-5.599259	1.671500	-0.683843
N	-3.392320	1.665756	-0.096607
C	-3.571597	2.534903	1.080405
C	-3.630782	4.025695	0.659236
O	-2.710806	4.814315	0.893005
C	-2.476182	2.309713	2.116148
N	-4.787557	4.336455	0.024356
C	-5.007832	5.625879	-0.591016

C	4.353165	4.261285	0.129050
C	4.667523	4.218298	1.620784
H	0.296615	-1.705764	1.110847
H	3.095549	0.978503	2.753297
H	2.414587	-0.657142	4.600336
H	-0.146701	-3.295464	3.357869
H	-0.002908	-2.334737	4.849999
H	1.326250	-3.406241	4.353409
H	1.295695	-5.547573	-0.291899
H	0.178891	-5.946213	1.050541
H	1.197123	-4.495112	1.146144
H	-2.432432	-3.596084	-4.067363
H	-2.096502	-5.055263	-3.094797
H	-2.167768	-3.046219	-1.608653
H	0.099473	-2.011481	-3.409483
H	-1.546094	-1.343068	-3.291401
H	0.545195	-4.209389	-1.879844
H	-0.803569	-4.307944	-4.071968
H	-2.812783	-1.054403	0.248549
H	-2.864553	-2.760668	0.489064
H	-4.561708	0.207229	1.306412
H	-6.149584	-0.370735	1.064061
H	-6.327623	-2.794670	1.373192
H	-5.932600	-4.784622	0.272527
H	-4.288487	-4.635697	0.958790
H	-4.638216	-4.022719	-0.687560
H	6.116068	-3.201381	1.539482
H	7.502401	-2.183916	1.086480
H	6.981401	-3.503728	0.016114
H	3.754319	-1.800833	1.122529
H	4.878191	0.401627	-2.284540
H	6.869827	-1.052501	-1.609669
H	-3.074027	0.011919	-2.022496
H	-4.094879	1.086383	-3.028106
H	-4.836178	-0.312486	-2.234152
H	-2.440262	1.496761	-0.424262
H	-2.761972	2.778012	3.068089
H	-1.549001	2.797139	1.785978
H	-4.559734	2.280331	1.498891
H	-5.991148	6.029446	-0.305528
H	-4.960202	5.562907	-1.690810
H	-4.223631	6.308605	-0.242118
H	-5.416264	3.558030	-0.196764
H	5.240457	5.108133	1.920283
H	5.262371	3.327815	1.874000
H	3.745211	4.187658	2.218933

H	5.262288	4.322638	-0.493939
H	3.778220	5.165214	-0.146340
H	-2.299068	1.238622	2.293140
O	0.180649	1.660188	-0.093417
H	0.145798	1.988415	0.819789
H	-0.424175	0.857277	-0.171081

Table S14. Optimized coordinates for model N803A CAD-bound, 5C.

Fe	2.030825	0.574997	-0.423276
N	1.578653	-0.012026	1.530840
O	0.937936	-0.737560	-1.489560
N	3.876297	-0.443101	-0.555776
C	2.884744	2.983785	-1.766346
O	2.254973	1.869381	-1.947302
O	3.129915	3.864461	-2.589291
C	3.367279	3.146229	-0.306850
O	3.071289	2.243291	0.486278
C	0.684368	-2.698824	3.949059
C	1.130063	-1.526299	3.146931
N	1.944494	-0.516091	3.640783
C	0.909850	-1.185892	1.832584
C	2.192523	0.371176	2.646965
C	0.681005	-5.101779	0.425263
C	-0.461711	-4.284685	-0.148802
O	-1.460878	-4.007105	0.547218
N	-0.298136	-3.880822	-1.430641
C	-1.301960	-3.183464	-2.236681
C	-1.699689	-4.072235	-3.421404
C	-0.788408	-1.808017	-2.707233
C	-0.326728	-0.902273	-1.558716
O	-1.173495	-0.406149	-0.762333
C	-4.982832	-4.143896	0.414388
N	-5.387796	-2.849292	0.956343
C	-4.597967	-1.761785	0.963428
N	-3.314349	-1.861045	0.614270
N	-5.119674	-0.582092	1.379132
C	6.679313	-2.660666	0.535828
C	5.672611	-1.739151	-0.071303
N	5.871092	-1.061173	-1.263961
C	4.420898	-1.341533	0.344798
C	4.777663	-0.295778	-1.519385
C	-4.079838	0.476132	-2.040490
C	-4.307640	1.367567	-0.842101
O	-5.446043	1.756002	-0.510516
N	-3.189908	1.699195	-0.138205

C	-3.202591	2.617610	1.012412
C	-3.370269	4.093173	0.545652
O	-2.441183	4.904736	0.586425
C	-1.934515	2.435256	1.837111
N	-4.632680	4.366964	0.124284
C	-5.008668	5.629408	-0.481690
C	4.167857	4.341052	0.097784
C	4.717732	4.260170	1.520063
H	0.298025	-1.691416	1.093735
H	2.815890	1.252760	2.750715
H	2.291242	-0.443793	4.593814
H	0.008183	-3.318656	3.344204
H	0.141805	-2.394513	4.858888
H	1.533742	-3.326640	4.264219
H	1.364692	-5.493350	-0.340407
H	0.262976	-5.939864	0.999258
H	1.259464	-4.476420	1.122482
H	-2.472547	-3.580971	-4.032302
H	-2.093622	-5.037420	-3.070142
H	-2.165929	-3.036042	-1.575147
H	0.050466	-1.947478	-3.405480
H	-1.604471	-1.311374	-3.256506
H	0.558379	-4.155713	-1.906219
H	-0.832846	-4.267592	-4.073078
H	-2.749253	-1.057784	0.314068
H	-2.807877	-2.762270	0.558633
H	-4.496345	0.220135	1.363535
H	-6.080253	-0.359402	1.129983
H	-6.265005	-2.791486	1.464977
H	-5.869723	-4.785536	0.371853
H	-4.217896	-4.632001	1.037574
H	-4.589450	-4.019457	-0.604439
H	6.279983	-3.084462	1.467127
H	7.618058	-2.136756	0.778487
H	6.928689	-3.497300	-0.136706
H	3.884032	-1.646510	1.237911
H	4.669629	0.333034	-2.397284
H	6.696394	-1.123899	-1.853706
H	-3.125374	-0.062634	-1.978062
H	-4.074103	1.100606	-2.948666
H	-4.918299	-0.227256	-2.132336
H	-2.289066	1.313743	-0.443684
H	-1.983679	3.051651	2.744898
H	-1.053182	2.756790	1.264502
H	-4.092742	2.369178	1.617498
H	-5.941815	6.007868	-0.037678

H	-5.152613	5.527929	-1.570159
H	-4.203234	6.351121	-0.297360
H	-5.254066	3.558209	0.009673
H	5.307403	5.158448	1.753735
H	5.367915	3.381228	1.643659
H	3.904330	4.184454	2.256526
H	4.964629	4.469906	-0.655486
H	3.521661	5.227215	-0.045804
H	-1.810242	1.382054	2.129462

Table S15. Optimized coordinates for model N803A CAD-unbound, 6C.

Fe	10.029343	1.649218	-0.370802
N	10.176877	0.849567	1.612174
O	9.505061	-0.108149	-1.311576
N	12.213239	1.393028	-0.569262
C	10.238226	4.139511	-1.814671
O	10.047812	2.877056	-2.002825
O	10.302381	5.037377	-2.657251
C	10.400276	4.493422	-0.322288
O	10.331811	3.562476	0.495387
C	10.489277	-2.036268	3.933629
C	10.431627	-0.759881	3.174109
N	10.855773	0.464723	3.670031
C	10.008097	-0.491463	1.893640
C	10.686371	1.404772	2.703896
C	11.371893	-4.119361	0.337787
C	9.970676	-3.837046	-0.188797
O	8.955802	-4.033197	0.512402
N	9.923663	-3.361540	-1.456891
C	8.704753	-3.214295	-2.250991
C	8.848704	-4.053849	-3.520835
C	8.390607	-1.746899	-2.607072
C	8.441624	-0.798093	-1.412269
O	7.457454	-0.755347	-0.605232
C	6.063318	-5.923293	0.371891
N	4.966621	-5.131899	0.918073
C	4.963750	-3.792098	0.869895
N	6.085870	-3.148972	0.519692
N	3.842987	-3.108948	1.182928
C	15.752557	0.673611	0.441739
C	14.418402	1.030219	-0.139969
N	14.259652	1.667917	-1.361268
C	13.130249	0.865899	0.325673
C	12.931568	1.867334	-1.580399
C	10.620551	5.910435	0.101021

C	10.832474	6.066852	1.603981
H	10.076091	-2.846443	3.316885
H	9.904627	-1.991095	4.867284
H	11.522687	-2.308263	4.204914
H	9.576681	-1.172212	1.167318
H	10.943772	2.452606	2.817819
H	11.227274	0.635030	4.600747
H	12.137549	-4.122295	-0.449485
H	11.367976	-5.095285	0.842604
H	11.641935	-3.358551	1.086122
H	7.896376	-3.612678	-1.622904
H	7.942485	-3.979215	-4.141377
H	9.016788	-5.113758	-3.277580
H	9.112363	-1.392132	-3.358055
H	7.385008	-1.717013	-3.055183
H	9.696540	-3.699450	-4.129679
H	10.806267	-3.215335	-1.940766
H	6.120122	-2.173807	0.203407
H	7.008914	-3.609248	0.513733
H	3.860104	-2.094311	1.182458
H	2.933365	-3.549770	1.088661
H	4.204200	-5.602163	1.394883
H	5.769077	-6.978222	0.404648
H	6.993062	-5.799065	0.947724
H	6.248859	-5.641973	-0.674793
H	15.611910	0.164830	1.404997
H	16.372626	1.567524	0.618232
H	16.320746	-0.002203	-0.217923
H	12.812025	0.398417	1.252126
H	12.529321	2.343415	-2.468714
H	15.006759	1.948572	-1.990238
H	11.470591	6.302733	-0.484961
H	9.755631	6.498070	-0.258134
H	10.984146	7.124849	1.863825
H	11.715414	5.502523	1.939721
H	9.963539	5.696860	2.167838
H	-38.587153	0.201605	0.003121
H	-38.882120	3.182659	-0.194201
H	-39.406075	2.076449	-1.501005
H	-40.294122	2.108064	0.051717
C	-39.297885	2.190610	-0.409602
N	-38.391802	1.199693	0.139765
H	-36.961240	-0.422293	1.563659
H	-34.449399	1.347870	1.245743
H	-34.497230	-0.258677	2.045815
H	-35.040238	-0.228562	-0.649794

C	-35.082188	0.640100	1.801420
O	-36.726405	2.667720	0.742718
C	-37.159081	1.516801	0.617978
C	-36.317963	0.265564	0.991771
N	-35.933348	-0.461809	-0.223687
H	-36.335424	-3.077725	-2.022614
H	-36.815835	-1.661568	-2.972440
H	-35.159468	-1.757039	-2.302542
O	-37.910522	-1.578119	-0.440938
C	-36.763359	-1.334058	-0.856406
C	-36.216364	-1.988222	-2.109361
H	-35.379749	1.132179	2.737518
O	7.882008	1.783702	0.041537
H	7.631106	2.103009	0.922954
H	7.570314	0.831135	-0.052507

Table S16. Optimized coordinates for model N803A CAD-unbound, 5C.

Fe	10.344482	1.611662	-0.396755
N	10.317332	0.921667	1.581847
O	9.672381	0.032857	-1.325343
N	12.447446	1.427478	-0.581495
C	10.298816	4.191106	-1.794650
O	10.205784	2.926942	-1.982091
O	10.247472	5.109289	-2.617337
C	10.513535	4.549654	-0.297250
O	10.487933	3.630823	0.527640
C	10.731507	-1.932107	3.937908
C	10.609927	-0.663298	3.168880
N	10.941446	0.586691	3.670203
C	10.216296	-0.427287	1.872304
C	10.750968	1.510717	2.690637
C	11.617933	-4.025817	0.349218
C	10.212601	-3.772683	-0.181668
O	9.201443	-4.007652	0.510494
N	10.160311	-3.272834	-1.441599
C	8.940339	-3.137745	-2.238886
C	9.094314	-3.978446	-3.509375
C	8.612913	-1.668972	-2.579248
C	8.645960	-0.750100	-1.353381
O	7.755740	-0.809807	-0.478896
C	6.312896	-5.840032	0.389962
N	5.198940	-5.051499	0.907003
C	5.209243	-3.709298	0.880731
N	6.342972	-3.076830	0.557865
N	4.090388	-3.019788	1.188417

C	15.989199	0.776127	0.436264
C	14.650895	1.097886	-0.149611
N	14.479377	1.669401	-1.403745
C	13.369873	0.953749	0.336500
C	13.152854	1.852000	-1.624141
C	10.743949	5.971573	0.099681
C	11.058579	6.163695	1.580415
H	10.353948	-2.765409	3.329211
H	10.149042	-1.908165	4.873560
H	11.778090	-2.152081	4.206078
H	9.835423	-1.132829	1.141841
H	10.943015	2.571904	2.807278
H	11.257037	0.786801	4.615239
H	12.385734	-4.017357	-0.436146
H	11.631819	-4.999158	0.858493
H	11.871643	-3.256396	1.094539
H	8.136556	-3.544808	-1.610566
H	8.187534	-3.914546	-4.130453
H	9.273350	-5.035805	-3.263032
H	9.328095	-1.294470	-3.326709
H	7.606279	-1.642443	-3.026807
H	9.938794	-3.616438	-4.118461
H	11.041726	-3.109184	-1.922158
H	6.410671	-2.101095	0.240848
H	7.255336	-3.556383	0.547388
H	4.119692	-2.005390	1.197810
H	3.178381	-3.449108	1.068558
H	4.436521	-5.522388	1.383230
H	6.010948	-6.893459	0.391064
H	7.221209	-5.732530	1.002271
H	6.539434	-5.540609	-0.643270
H	15.859187	0.319423	1.426580
H	16.608572	1.679417	0.558757
H	16.552554	0.067427	-0.192134
H	13.057813	0.540145	1.290458
H	12.738144	2.285989	-2.528295
H	15.222128	1.916823	-2.052035
H	11.540396	6.364061	-0.556986
H	9.846308	6.535954	-0.213887
H	11.215535	7.228975	1.803419
H	11.969583	5.616574	1.865735
H	10.235374	5.798742	2.211930
H	-38.347057	0.196957	0.005435
H	-38.651351	3.176180	-0.205349
H	-39.173506	2.062354	-1.506373
H	-40.059612	2.098274	0.047352

C	-39.064247	2.181842	-0.415643
N	-38.154411	1.196244	0.137128
H	-36.715863	-0.414890	1.565427
H	-34.210625	1.361889	1.233549
H	-34.250720	-0.241423	2.040581
H	-34.800411	-0.226322	-0.653260
C	-34.839453	0.654223	1.793801
O	-36.491709	2.671842	0.729001
C	-36.921461	1.519132	0.610877
C	-36.075923	0.272109	0.988787
N	-35.691974	-0.459893	-0.224093
H	-36.087930	-3.086253	-2.007468
H	-36.578550	-1.678460	-2.964435
H	-34.919553	-1.761474	-2.299315
O	-37.666449	-1.582839	-0.431456
C	-36.520898	-1.337581	-0.850659
C	-35.974659	-1.996707	-2.101317
H	-35.136511	1.149232	2.728515

Table S17. Optimized coordinates for model N803A CAD-unbound, FIH R238 Moved to CS2/TauD position, 6C.

Fe	9.464281	-0.253523	-0.738789
N	9.370087	1.319148	-2.128232
O	9.495922	0.654879	1.101910
N	11.618679	-0.272709	-0.782465
C	9.323940	-3.200189	-0.874669
O	9.412020	-2.231098	-0.031740
O	9.369534	-4.418133	-0.609727
C	9.200742	-2.718051	-2.308982
O	9.285777	-1.492261	-2.482307
O	7.292373	-0.343183	-0.503481
C	9.723865	4.883648	-3.125949
C	9.616872	3.413533	-2.931596
N	9.858368	2.481921	-3.930681
C	9.307736	2.666551	-1.817779
C	9.698499	1.239425	-3.414389
C	10.639732	5.274894	1.003972
C	9.452189	4.419318	1.407915
O	8.406157	4.408372	0.740450
N	9.627285	3.663224	2.525686
C	8.563637	2.888507	3.156873
C	8.188783	3.533859	4.499825
C	8.965433	1.396467	3.328831
C	8.682423	0.550724	2.084371

O	7.649379	-0.182312	2.098472
C	15.090950	1.068643	-1.156558
C	13.789609	0.366326	-0.939889
N	13.697920	-0.926704	-0.445494
C	12.480506	0.750415	-1.137407
C	12.387167	-1.271987	-0.366045
C	9.081957	-3.674516	-3.449755
C	10.234354	-3.436954	-4.436222
C	-39.904723	-1.858665	-0.470504
N	-38.974774	-0.749541	-0.570600
C	-35.606829	0.346287	-1.787204
O	-37.293858	-1.906138	-1.633255
C	-37.726171	-0.882480	-1.092527
C	-36.866451	0.401117	-0.930885
N	-36.518293	0.595952	0.481505
O	-38.495145	1.577677	1.055541
C	-37.364196	1.171215	1.377979
C	-36.857648	1.279568	2.802469
N	10.354264	-4.496907	2.009225
C	9.671059	-3.755569	2.889608
N	8.605127	-3.045453	2.463311
N	10.022348	-3.728953	4.183263
C	11.276702	-4.290609	4.616867
H	9.426221	5.391651	-2.198730
H	9.065502	5.243077	-3.933540
H	10.752513	5.193857	-3.372841
H	9.017772	3.023731	-0.832325
H	9.824415	0.320711	-3.975709
H	10.095796	2.691281	-4.896544
H	11.459671	5.275314	1.736679
H	10.295313	6.307822	0.852475
H	11.031040	4.913433	0.040818
H	7.707438	2.965312	2.470838
H	7.334421	3.012076	4.957611
H	7.913405	4.588568	4.353100
H	10.034446	1.337397	3.590552
H	8.381728	0.972062	4.158081
H	9.031345	3.491534	5.210645
H	10.497494	3.762435	3.042346
H	14.907153	2.078279	-1.547849
H	15.727887	0.536758	-1.881815
H	15.662745	1.169125	-0.219822
H	12.105074	1.699959	-1.507478
H	12.034025	-2.226069	0.010898
H	14.481379	-1.521123	-0.189186
H	9.078460	-4.701801	-3.062891

H	8.115183	-3.494641	-3.951676
H	10.151229	-4.120897	-5.293674
H	11.209473	-3.612544	-3.956769
H	10.216816	-2.405436	-4.815179
H	-39.168917	0.122548	-0.065935
H	-39.497853	-2.693604	-1.054380
H	-40.034817	-2.183391	0.575348
H	-40.889395	-1.579497	-0.875836
H	-37.486857	1.267670	-1.210363
H	-34.995206	-0.530989	-1.529215
H	-35.010630	1.260274	-1.650312
H	-35.641025	0.200264	0.808945
H	-36.985528	2.315693	3.146818
H	-37.477310	0.640979	3.450072
H	-35.804210	0.989484	2.920898
H	-35.876477	0.256512	-2.848418
H	6.795452	0.445543	-0.778595
H	7.247942	-0.384108	0.506951
H	8.266617	-2.276145	3.041124
H	8.662534	-2.768776	1.467122
H	11.006411	-5.201399	2.335770
H	9.986799	-4.574497	1.035572
H	9.541022	-3.078468	4.794908
H	11.422732	-4.046599	5.675127
H	12.126376	-3.883229	4.044826
H	11.277909	-5.389684	4.534441

Table S18. Optimized coordinates for model N803A CAD-unbound, FIH R238 Moved to CS2/TauD position, 5C.

Fe	9.721178	-0.204164	-0.703851
N	9.554857	1.324409	-2.105257
O	9.594673	0.735438	1.023286
N	11.830302	-0.310729	-0.777651
C	9.522280	-3.155249	-0.950942
O	9.575540	-2.194247	-0.101745
O	9.614484	-4.373124	-0.708829
C	9.350411	-2.657347	-2.385905
O	9.375926	-1.430983	-2.537958
C	9.923235	4.887420	-3.110642
C	9.801996	3.419123	-2.909821
N	10.020551	2.487467	-3.913829
C	9.504453	2.673061	-1.792074
C	9.860319	1.245738	-3.398570
C	10.840976	5.246122	1.021789
C	9.640043	4.409373	1.424810

O	8.586011	4.438071	0.771152
N	9.815704	3.625111	2.522139
C	8.748273	2.850269	3.146981
C	8.390707	3.479165	4.504965
C	9.133888	1.356540	3.304459
C	8.883798	0.469724	2.075358
O	8.041012	-0.445772	2.150273
C	15.289276	1.054580	-1.173395
C	13.995483	0.341786	-0.946273
N	13.912145	-0.941667	-0.424047
C	12.685008	0.711230	-1.154813
C	12.605311	-1.295963	-0.337584
C	9.233247	-3.607521	-3.533372
C	10.429070	-3.422967	-4.485886
C	-39.707560	-1.851003	-0.486542
N	-38.773552	-0.744618	-0.578786
C	-35.399183	0.346129	-1.781947
O	-37.094142	-1.901388	-1.643695
C	-37.524229	-0.879117	-1.098583
C	-36.660558	0.400685	-0.928233
N	-36.315104	0.586948	0.485980
O	-38.289889	1.572702	1.060288
C	-37.161146	1.160625	1.383340
C	-36.657508	1.260231	2.809485
N	10.576132	-4.512855	1.947453
C	9.868727	-3.798304	2.837452
N	8.800625	-3.092737	2.419214
N	10.216256	-3.792486	4.130456
C	11.474790	-4.347525	4.559847
H	9.642829	5.402811	-2.182143
H	9.258547	5.251013	-3.911067
H	10.952369	5.184026	-3.371639
H	9.226415	3.026194	-0.802036
H	9.969340	0.329201	-3.965914
H	10.240892	2.697154	-4.883587
H	11.666131	5.223682	1.748514
H	10.515931	6.286993	0.882752
H	11.219604	4.887197	0.052473
H	7.889830	2.946722	2.466461
H	7.532272	2.961678	4.960182
H	8.129040	4.540109	4.378808
H	10.199609	1.292164	3.586217
H	8.545620	0.929642	4.129146
H	9.237789	3.412471	5.208615
H	10.695103	3.695280	3.027717
H	15.094105	2.056171	-1.579266

H	15.932028	0.518838	-1.890532
H	15.858940	1.174135	-0.237745
H	12.303731	1.650636	-1.543656
H	12.259693	-2.243888	0.061791
H	14.699779	-1.523767	-0.151999
H	9.179320	-4.634550	-3.150186
H	8.295106	-3.382759	-4.068533
H	10.336388	-4.106899	-5.341764
H	11.379955	-3.642277	-3.977366
H	10.468541	-2.393115	-4.868096
H	-38.965904	0.125561	-0.070157
H	-39.301917	-2.684532	-1.073275
H	-39.841637	-2.180232	0.557395
H	-40.690161	-1.566569	-0.893244
H	-37.277406	1.270782	-1.204555
H	-34.791355	-0.534859	-1.527662
H	-34.799986	1.257141	-1.638450
H	-35.440081	0.186421	0.813559
H	-36.779444	2.295863	3.157501
H	-37.282975	0.623292	3.453094
H	-35.606274	0.962873	2.929430
H	-35.666762	0.263492	-2.844257
H	8.511151	-2.267515	2.952591
H	8.830270	-2.841416	1.418685
H	11.175261	-5.265313	2.270467
H	10.223362	-4.563424	0.969696
H	9.672460	-3.225593	4.772211
H	11.641018	-4.072206	5.607446
H	12.311307	-3.953690	3.960926
H	11.478553	-5.448990	4.506281

Table S19. Optimized coordinates for model N803A CAD-unbound, FIH N205 and N294 added, 5C.

Fe	-8.508354	-0.055263	-0.987185
N	-8.400014	-1.605268	-2.385471
O	-7.855069	-0.878644	0.656779
N	-10.611098	-0.139345	-0.755632
C	-8.540184	2.878190	-0.976741
O	-8.388922	1.873217	-0.208227
O	-8.580867	4.086578	-0.669775
C	-8.725358	2.481254	-2.454607
O	-8.693542	1.273133	-2.718663
C	-8.683490	-5.250482	-3.095360
C	-8.620219	-3.764520	-3.016666
N	-9.027729	-2.917986	-4.038125

C	-8.224176	-2.924309	-2.001859
C	-8.879680	-1.633835	-3.624893
C	-9.617514	-5.413899	1.045773
C	-8.237790	-4.882313	1.413439
O	-7.199394	-5.385555	0.939640
N	-8.238684	-3.839671	2.281933
C	-7.049002	-3.289603	2.933931
C	-7.198484	-3.456711	4.448327
C	-6.807973	-1.814043	2.559322
C	-6.839051	-1.576462	1.046626
O	-5.959530	-2.057775	0.302402
C	-4.274121	-6.857472	1.940352
N	-3.168666	-6.375581	1.119215
C	-3.205613	-5.181824	0.508692
N	-4.358495	-4.500572	0.487021
N	-2.095141	-4.690586	-0.079839
C	-14.091072	-1.374270	-1.371395
C	-12.786842	-0.736130	-1.009071
N	-12.683004	0.423749	-0.253745
C	-11.482151	-1.068801	-1.300867
C	-11.371940	0.750627	-0.124718
C	-8.948458	3.530689	-3.491218
C	-9.253433	2.977490	-4.879327
H	-8.254438	-5.683363	-2.181326
H	-8.115030	-5.643714	-3.953856
H	-9.720517	-5.611717	-3.191547
H	-7.789977	-3.177606	-1.039900
H	-9.134466	-0.765391	-4.222697
H	-9.363324	-3.207477	-4.952886
H	-10.431846	-4.949448	1.617987
H	-9.632617	-6.499876	1.216142
H	-9.798377	-5.245798	-0.026227
H	-6.208613	-3.891512	2.563937
H	-6.316251	-3.059006	4.973355
H	-7.314938	-4.516867	4.719011
H	-7.568557	-1.180281	3.039417
H	-5.821515	-1.520096	2.953322
H	-8.080268	-2.907110	4.816599
H	-9.138580	-3.503119	2.615709
H	-4.445144	-3.499100	0.285403
H	-5.263601	-4.939108	0.713528
H	-2.142135	-3.810862	-0.583400
H	-1.176669	-4.989124	0.232721
H	-2.381531	-6.989686	0.937492
H	-3.955289	-7.788584	2.421974
H	-5.177478	-7.060941	1.345592

H	-4.515871	-6.121876	2.720614
H	-13.908032	-2.286065	-1.955637
H	-14.717292	-0.702098	-1.979941
H	-14.672000	-1.654617	-0.478041
H	-11.119958	-1.918428	-1.871409
H	-11.015433	1.612288	0.434479
H	-13.459407	0.951874	0.135865
H	-9.749011	4.191787	-3.114756
H	-8.051576	4.178260	-3.488526
H	-9.410864	3.800219	-5.591437
H	-10.162127	2.357378	-4.867082
H	-8.425483	2.356527	-5.251278
H	40.111998	0.088012	-0.108469
H	40.472525	2.861489	-1.200978
H	41.031138	2.398261	0.435557
H	41.847188	1.728918	-1.009051
C	40.875464	2.039989	-0.595732
N	39.924130	0.945513	-0.639793
H	38.390200	-1.066210	-1.184323
H	35.927517	0.768224	-1.523673
H	35.904373	-1.026479	-1.575007
H	36.603290	0.104932	0.830885
C	36.516164	-0.131075	-1.758276
O	38.246574	2.092346	-1.718464
C	38.669792	1.081810	-1.146718
C	37.790591	-0.179260	-0.924005
N	37.466364	-0.318739	0.500594
H	37.949337	-1.959022	3.211674
H	38.481119	-0.286252	3.451666
H	36.791594	-0.616131	2.963993
O	39.435285	-1.318538	1.070903
C	38.318299	-0.880126	1.400151
C	37.836523	-0.931965	2.836288
H	36.767259	-0.088079	-2.826888
N	-6.381160	5.663856	0.596381
C	-6.188471	7.012633	0.572741
O	-5.246429	7.558406	1.159336
C	-7.230590	7.802696	-0.223329
C	-6.698464	9.153502	-0.706755
H	-7.200135	5.202221	0.190966
H	-5.781120	5.116560	1.206807
H	-7.600664	7.191681	-1.063056
H	-8.098188	7.956040	0.443616
H	-7.498004	9.740192	-1.183732
H	-5.885712	9.023276	-1.438055
H	-6.295245	9.728579	0.138264

N	-9.767610	3.542415	2.037064
O	-10.950592	5.400148	2.629835
C	-10.476389	4.299060	2.926016
C	-10.704376	3.661141	4.300475
C	-10.691138	4.703412	5.421942
H	-9.241386	2.730085	2.343273
H	-9.460019	3.954623	1.149304
H	-11.691280	3.165442	4.267521
H	-9.963813	2.866623	4.490129
H	-10.972619	4.249873	6.384089
H	-11.398874	5.511957	5.191869
H	-9.692561	5.153162	5.534647

Table S20. Optimized coordinates for model N803A* CAD-bound, 6C.

Fe	2.101875	0.555681	-0.483331
N	1.619209	-0.273300	1.530020
O	0.928854	-0.821525	-1.494765
N	3.860313	-0.595876	-0.606622
C	3.482580	2.747829	-1.768194
O	2.783356	1.702338	-2.047430
O	3.993008	3.559066	-2.542979
C	3.674238	2.944778	-0.246346
O	3.135959	2.123813	0.512328
C	0.384569	-2.804094	4.007124
C	0.983253	-1.713659	3.169945
N	1.907617	-0.797703	3.654446
C	0.819457	-1.361599	1.844879
C	2.260430	0.044423	2.649034
C	0.401498	-5.154625	0.448132
C	-0.687952	-4.284276	-0.152489
O	-1.688240	-3.952193	0.518560
N	-0.473906	-3.891709	-1.430567
C	-1.421376	-3.143405	-2.257450
C	-1.857401	-4.004732	-3.437791
C	-0.815273	-1.820125	-2.752238
C	-0.322595	-0.941934	-1.613089
O	-1.189635	-0.399768	-0.838954
C	-5.232640	-4.042706	0.317724
N	-5.599992	-2.756305	0.895120
C	-4.797150	-1.680226	0.911767
N	-3.521146	-1.777002	0.532045
N	-5.310254	-0.513285	1.371029
C	6.458862	-2.879588	0.737786
C	5.562609	-1.939008	0.023712
N	5.908511	-1.234387	-1.116307

C	4.283309	-1.532966	0.313608
C	4.861534	-0.438916	-1.464321
C	-4.146936	0.586254	-2.044582
C	-4.311405	1.477186	-0.833816
O	-5.431740	1.818635	-0.403541
N	-3.157615	1.852048	-0.214327
C	-3.131445	2.729373	0.965368
C	-3.334950	4.210692	0.548288
O	-2.415150	5.033895	0.576175
C	-1.832069	2.588348	1.748380
N	-4.606204	4.474778	0.163816
C	-4.974212	5.739655	-0.430196
C	4.478329	4.094762	0.266654
C	4.660918	4.077049	1.780309
H	0.158083	-1.806981	1.108990
H	2.975683	0.853715	2.756219
H	2.260709	-0.757519	4.606841
H	-0.320726	-3.385100	3.397002
H	-0.164594	-2.400000	4.872890
H	1.154911	-3.492252	4.390428
H	1.067261	-5.597614	-0.305073
H	-0.067011	-5.956256	1.034709
H	1.009450	-4.547393	1.136514
H	-2.586566	-3.467357	-4.063333
H	-2.320068	-4.942206	-3.094302
H	-2.279573	-2.924094	-1.609086
H	0.025694	-2.024106	-3.431324
H	-1.589036	-1.280385	-3.321045
H	0.375174	-4.216635	-1.888036
H	-0.995972	-4.260329	-4.075985
H	-2.954978	-0.957141	0.298712
H	-3.006054	-2.674878	0.477151
H	-4.707912	0.303214	1.360683
H	-6.279494	-0.294963	1.152951
H	-6.467398	-2.694720	1.419748
H	-6.133427	-4.664214	0.270696
H	-4.470433	-4.562685	0.918361
H	-4.848510	-3.902827	-0.702787
H	5.933772	-3.305020	1.603827
H	7.369170	-2.380480	1.109580
H	6.782741	-3.717304	0.097923
H	3.647661	-1.858576	1.130070
H	4.855443	0.218587	-2.326898
H	6.792548	-1.295689	-1.613379
H	-3.178440	0.069247	-2.049142
H	-4.225899	1.201876	-2.955356

H	-4.971056	-0.138867	-2.067850
H	-2.272503	1.608220	-0.658245
H	-1.979049	2.957420	2.773577
H	-1.070705	3.237331	1.294372
H	-3.994708	2.438218	1.586071
H	-5.924077	6.102124	-0.009400
H	-5.084243	5.658131	-1.524655
H	-4.182321	6.465509	-0.209702
H	-5.231795	3.668460	0.061798
H	5.254617	4.943248	2.107204
H	5.181185	3.163639	2.105746
H	3.690543	4.112773	2.296909
H	5.441029	4.092497	-0.274035
H	3.981111	5.019653	-0.080038
H	-1.502752	1.540863	1.810797
O	0.296863	1.673892	-0.325310
H	0.208506	2.176877	0.498601
H	-0.373744	0.919292	-0.328522

Table S21. Optimized coordinates for model N803A* CAD-bound, 5C.

Fe	2.018288	0.543360	-0.429639
N	1.585352	-0.085509	1.520235
O	0.927445	-0.743153	-1.522032
N	3.870556	-0.461106	-0.572683
C	2.869953	2.978440	-1.734539
O	2.252126	1.861753	-1.936501
O	3.106789	3.878358	-2.539515
C	3.352762	3.115855	-0.272707
O	3.052796	2.201558	0.506167
C	0.646760	-2.766092	3.930891
C	1.125347	-1.608129	3.125816
N	2.017925	-0.656625	3.600421
C	0.865215	-1.227082	1.829250
C	2.269823	0.237434	2.614116
C	0.595397	-5.129356	0.380678
C	-0.533971	-4.285141	-0.180699
O	-1.521431	-3.989152	0.524744
N	-0.372327	-3.880013	-1.462085
C	-1.365791	-3.155217	-2.256792
C	-1.795447	-4.029616	-3.440240
C	-0.821168	-1.792587	-2.727672
C	-0.339051	-0.900322	-1.577974
O	-1.173437	-0.406436	-0.767651
C	-5.056949	-4.106495	0.413827
N	-5.438379	-2.817328	0.980892

C	-4.641432	-1.735245	0.986998
N	-3.363927	-1.835559	0.616466
N	-5.157457	-0.560439	1.423083
C	6.622031	-2.758522	0.483096
C	5.646968	-1.787152	-0.096906
N	5.919646	-0.985683	-1.194978
C	4.362545	-1.445975	0.265559
C	4.835743	-0.206856	-1.448001
C	-4.114900	0.530084	-1.994804
C	-4.255644	1.423901	-0.782685
O	-5.371381	1.815635	-0.381394
N	-3.095977	1.760206	-0.153837
C	-3.045101	2.695259	0.983200
C	-3.263950	4.156148	0.505366
O	-2.337603	4.968608	0.426974
C	-1.720753	2.582365	1.721229
N	-4.562994	4.424793	0.221121
C	-4.975347	5.675877	-0.373499
C	4.158912	4.300125	0.151609
C	4.746037	4.172872	1.555640
H	0.190260	-1.679929	1.110669
H	2.945623	1.080911	2.705547
H	2.414423	-0.627904	4.536104
H	-0.060174	-3.358245	3.333492
H	0.128434	-2.444490	4.848929
H	1.476268	-3.426215	4.232296
H	1.278022	-5.513838	-0.389395
H	0.164105	-5.973705	0.935551
H	1.176848	-4.525306	1.094021
H	-2.561588	-3.518049	-4.042864
H	-2.209203	-4.986563	-3.089105
H	-2.219438	-2.986520	-1.587072
H	0.012344	-1.949742	-3.428545
H	-1.626791	-1.275523	-3.273769
H	0.472427	-4.174547	-1.946860
H	-0.939085	-4.243265	-4.100166
H	-2.797163	-1.028551	0.333704
H	-2.859034	-2.737235	0.548322
H	-4.547388	0.250982	1.409922
H	-6.124527	-0.342152	1.196668
H	-6.307234	-2.758023	1.503375
H	-5.951300	-4.737901	0.374528
H	-4.288364	-4.612995	1.017678
H	-4.676916	-3.971043	-0.608698
H	6.164048	-3.279428	1.334735
H	7.533334	-2.255362	0.845060

H	6.931101	-3.519398	-0.251820
H	3.766120	-1.848554	1.078783
H	4.780852	0.505665	-2.264746
H	6.786699	-0.976453	-1.725273
H	-3.166884	-0.023810	-1.989963
H	-4.153471	1.156379	-2.900749
H	-4.967263	-0.160973	-2.035236
H	-2.218684	1.346196	-0.488783
H	-1.742785	3.207380	2.624350
H	-0.897902	2.943882	1.088983
H	-3.884129	2.439395	1.653820
H	-5.889690	6.050239	0.111078
H	-5.170200	5.569989	-1.454210
H	-4.168073	6.405136	-0.232877
H	-5.185829	3.611858	0.157103
H	5.333447	5.067803	1.807156
H	5.407579	3.296739	1.630179
H	3.952754	4.061575	2.309199
H	4.933390	4.462223	-0.617782
H	3.502663	5.186005	0.058684
H	-1.520370	1.542029	2.017288

Table S22. Optimized coordinates for model N803A* CAD-unbound, 6C.

Fe	10.018664	1.649769	-0.368889
N	10.168540	0.848591	1.613255
O	9.495753	-0.107224	-1.311344
N	12.202460	1.395935	-0.569590
C	10.223677	4.141701	-1.810772
O	10.034376	2.879199	-1.999737
O	10.286155	5.040297	-2.652690
C	10.386568	4.494455	-0.318232
O	10.319826	3.562570	0.498549
C	10.487657	-2.039403	3.931105
C	10.427400	-0.762215	3.173130
N	10.850401	0.462448	3.669901
C	10.001965	-0.492987	1.893469
C	10.678521	1.403326	2.704993
C	11.369270	-4.117754	0.332276
C	9.967165	-3.836880	-0.192748
O	8.953189	-4.035246	0.509116
N	9.918351	-3.359798	-1.460192
C	8.698434	-3.213402	-2.252930
C	8.842112	-4.051535	-3.523734
C	8.381860	-1.746074	-2.607221
C	8.433071	-0.798406	-1.411506

O	7.449797	-0.757736	-0.603283
C	6.063011	-5.928422	0.369902
N	4.965948	-5.138946	0.918143
C	4.961305	-3.799117	0.871173
N	6.082213	-3.154267	0.520292
N	3.840035	-3.117635	1.186101
C	15.743992	0.680635	0.436653
C	14.408601	1.035461	-0.143320
N	14.247405	1.672127	-1.364870
C	13.121302	0.870305	0.324351
C	12.918847	1.870196	-1.582127
C	10.605659	5.911262	0.106314
C	10.818281	6.066489	1.609295
H	10.075078	-2.849429	3.313761
H	9.903823	-1.996203	4.865366
H	11.521717	-2.310218	4.201096
H	9.570631	-1.173515	1.166891
H	10.934759	2.451362	2.819703
H	11.222879	0.632240	4.600324
H	12.133991	-4.119830	-0.455893
H	11.366941	-5.093698	0.837042
H	11.639369	-3.356666	1.080308
H	7.891270	-3.613492	-1.624374
H	7.935155	-3.977369	-4.143252
H	9.011727	-5.111478	-3.281709
H	9.102154	-1.389566	-3.358783
H	7.375641	-1.717188	-3.054010
H	9.688883	-3.695508	-4.133110
H	10.800311	-3.212076	-1.944794
H	6.114836	-2.178753	0.204976
H	7.005830	-3.613362	0.512933
H	3.856045	-2.102973	1.186384
H	2.930878	-3.559469	1.092030
H	4.204826	-5.610610	1.395643
H	5.770136	-6.983753	0.402001
H	6.993280	-5.803540	0.944736
H	6.246914	-5.645877	-0.676739
H	15.605330	0.172278	1.400427
H	16.363356	1.575312	0.611717
H	16.311927	0.005034	-0.223436
H	12.804926	0.403129	1.251585
H	12.514695	2.345492	-2.470001
H	14.993317	1.953037	-1.995132
H	11.455013	6.304948	-0.479747
H	9.739979	6.498393	-0.251836
H	10.969115	7.124391	1.870007

H	11.701948	5.502684	1.944004
H	9.950017	5.695179	2.173309
H	-38.565041	0.161945	0.097953
H	-38.913827	3.132206	-0.157083
H	-39.429508	2.006348	-1.447633
H	-40.298489	2.028542	0.114547
C	-39.309148	2.129002	-0.357697
N	-38.380275	1.166941	0.189865
H	-36.857721	-0.366771	1.586570
H	-34.436902	1.489987	1.119515
H	-34.382567	-0.076554	1.994699
H	-35.017182	-0.216605	-0.701752
C	-35.019689	0.778003	1.721859
O	-36.703137	2.684614	0.592690
C	-37.126555	1.523361	0.566389
C	-36.251502	0.311341	0.965370
N	-35.884469	-0.459358	-0.229817
H	-36.357604	-3.129854	-1.956677
H	-36.843316	-1.720484	-2.915039
H	-35.169880	-1.831824	-2.291798
O	-37.850941	-1.610248	-0.337498
C	-36.725530	-1.361740	-0.806079
C	-36.224079	-2.044221	-2.064779
H	-35.320762	1.298219	2.641419
O	7.871460	1.781375	0.044879
H	7.620718	2.100062	0.926560
H	7.560863	0.828503	-0.049454

Table S23. Optimized coordinates for model N803A* CAD-unbound, 5C.

Fe	10.334141	1.612201	-0.395184
N	10.309558	0.920106	1.582780
O	9.662750	0.033486	-1.324451
N	12.437129	1.430211	-0.581963
C	10.285794	4.193086	-1.790347
O	10.193360	2.929055	-1.979018
O	10.233632	5.112061	-2.612090
C	10.500978	4.550256	-0.292617
O	10.476509	3.630556	0.531311
C	10.729721	-1.935575	3.935516
C	10.605596	-0.666129	3.167923
N	10.935751	0.583790	3.670295
C	10.210550	-0.429286	1.871923
C	10.743240	1.508589	2.691853
C	11.615166	-4.024356	0.343678
C	10.209011	-3.772206	-0.185507

O	9.198819	-4.008919	0.507472
N	10.154868	-3.271188	-1.444901
C	8.933884	-3.136826	-2.240783
C	9.087724	-3.975834	-3.512427
C	8.603841	-1.668148	-2.579146
C	8.637076	-0.750443	-1.352363
O	7.747701	-0.811912	-0.477144
C	6.312345	-5.844961	0.387565
N	5.198042	-5.058336	0.906776
C	5.206589	-3.716103	0.881759
N	6.339205	-3.081897	0.558435
N	4.087150	-3.028286	1.191154
C	15.980695	0.782719	0.431806
C	14.641387	1.102941	-0.152568
N	14.467840	1.673881	-1.406695
C	13.361089	0.957616	0.335063
C	13.140882	1.855161	-1.625551
C	10.730325	5.971968	0.105615
C	11.044745	6.163099	1.586523
H	10.352718	-2.768746	3.326283
H	10.148143	-1.913425	4.871764
H	11.776879	-2.154357	4.202391
H	9.829991	-1.134551	1.141028
H	10.933871	2.569923	2.809478
H	11.251758	0.783342	4.615310
H	12.382086	-4.014539	-0.442519
H	11.630556	-4.998081	0.852177
H	11.868917	-3.255265	1.089333
H	8.131356	-3.545811	-1.612106
H	8.180234	-3.912426	-4.132511
H	9.268449	-5.033235	-3.267514
H	9.317452	-1.291787	-3.327190
H	7.596568	-1.642711	-3.025331
H	9.931087	-3.611936	-4.121931
H	11.035620	-3.106121	-1.926197
H	6.405364	-2.105760	0.242345
H	7.252163	-3.560280	0.546614
H	4.115257	-2.013848	1.200963
H	3.175584	-3.458597	1.071409
H	4.436686	-5.530642	1.383290
H	6.011746	-6.898777	0.388097
H	7.221308	-5.736857	0.998804
H	6.537151	-5.544293	-0.645685
H	15.852346	0.326351	1.422495
H	16.599375	1.686642	0.553142
H	16.543950	0.074261	-0.196953

H	13.050557	0.544037	1.289530
H	12.724672	2.288614	-2.529272
H	15.209589	1.921937	-2.055882
H	11.526542	6.365564	-0.550681
H	9.832320	6.535977	-0.207575
H	11.200983	7.228304	1.810389
H	11.956088	5.616345	1.871462
H	10.221741	5.797107	2.217700
H	-38.327489	0.159198	0.097602
H	-38.681414	3.127846	-0.168707
H	-39.195444	1.996073	-1.454717
H	-40.064189	2.022921	0.107514
C	-39.075100	2.123198	-0.365288
N	-38.144529	1.164844	0.185907
H	-36.618937	-0.361308	1.587211
H	-34.201802	1.498665	1.114016
H	-34.144174	-0.064958	1.994295
H	-34.778524	-0.215711	-0.701507
C	-34.783057	0.787387	1.718665
O	-36.469679	2.686822	0.581992
C	-36.891188	1.524783	0.560395
C	-36.013935	0.315779	0.963714
N	-35.645448	-0.458302	-0.228826
H	-36.113336	-3.135347	-1.946647
H	-36.602241	-1.730354	-2.909779
H	-34.928477	-1.835916	-2.286416
O	-37.609850	-1.613092	-0.332673
C	-36.484910	-1.364060	-0.802102
C	-35.982184	-2.049801	-2.058496
H	-35.085246	1.309958	2.636521

Table S24. Optimized coordinates for water.

O	0.000000	0.118232	0.000000
H	0.770510	-0.472945	0.000000
H	-0.770510	-0.472913	0.000000

References

1. Gaussian 09, Revision **C.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
2. J. M. Elkins, K. S. Hewitson, L. A. McNeill, J. F. Seibel, I. Schlemminger, C. W. Pugh, P. J. Ratcliffe, and C. J. Schofield, *J. Biol. Chem.* 2003, **278**, 1802–1806.
3. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098–3100.
4. J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822–8824.
5. K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650–654.
6. A. J. H. Wachters, *J. Chem. Phys.*, 1970, **52**, 1033.
7. P. J. Hay, *J. Chem. Phys.*, 1977, **66**, 4377–4384.
8. K. Raghavachari and G. W. Trucks, *J. Chem. Phys.*, 1989, **91**, 1062–1065.
9. R. Ditchfield, W. J. Hehre, and J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724.
10. W. J. Hehre, R. Ditchfield, and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257.
11. P. C. Hariharan and J. A. Pople, *Theor. Chem. Acc.*, 1973, **28**, 213–222.
12. P. C. Hariharan and J. A. Pople, *Mol. Phys.*, 1974, **27**, 209–214.
13. M. S. Gordon, *Chem. Phys. Lett.*, 1980, **76**, 163–168.
14. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999–3093.